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MCNPX, VERSION 2.5.c

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MCNPX, VERSION 2.5.c

Abstract

MCNPX is a Fortran90 Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. These capabilities are summarized, along with their quality guarantee and code availability. The user interface changes from MCNP then are described. Finally, the new capabilities of the latest version, MCNPX 2.5.c, are documented. Future plans and references also are provided.

1.0. INTRODUCTION

MCNPX is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports all particles at all energies. MCNPX stands for MCNP eXtended. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed: it can be used with confidence. MCNPX is available from the Radiation Safety Information and Computational Center (RSICC) and the Office of Economic Community Development (OECD)/Nuclear Energy Agency (NEA); beta test program versions may be downloaded from the MCNPX website at http://mcnpx.lanl.gov.

1.1. MCNPX Capabilities beyond MCNP4C3

Each successive version of MCNPX adds new capabilities and modernizes the code for new hardware, operating systems, and compilers. The capabilities of MCNPX beyond MCNP4C3 now are listed and are grouped according to the MCNPX version. Initials of principal developers are shown in parentheses.[1] For completeness we also list the capabilities and principal developers of MCNP and MCNPX since MCNP4B.

MCNPX 2.5.c (April 2003)

- message passing interface (MPI) multiprocessing (JL/GWM);
- i,j,k lattice indexing in geometry plots (JSH),

[1] Kenneth J. Adams (KJA), Leland L. Carter (LLC), Skip Egdorf (HWE), Thomas M. Evans (TME), Jeffrey A. Favorite (JAF), Franz X. Gallmeier (FXG), John S. Hendricks (JSH), H. Grady Hughes (HGH), Julian Lebenhaft (JL), Robert C. Little (RCL), Stepan G. Mashnik (SGM), Gregg W. McKinney (GWM), Richard E. Prael (REP), Teresa L. Roberts (TLR), Arnold J. Sierk (AJS), Edward C. Snow (ECS), Laurie S. Waters (LSW), Christopher J. Werner (CJW), and Morgan C. White (MCW).

- enablement of weight-window generator in physics model region (FXG/JSH);
- enablement of exponential transform in physics model region (FXG/JSH);
- extension of neutron model physics below 20 MeV (JSH);
- ^{3}He coincidence detector modeling (HGH/JSH);
- F90 autoconfiguration (TLR);
- corrections/enhancements/extensions.

MCNPX 2.5.b (November 2002)

- CEM2k physics (SGM/AJS/FXG);
- mix and match (JSH);
- positron sources (HGH);
- spontaneous fission (JSH);
- corrections/enhancements/extensions.

MCNPX 2.4.0 (August 2002)

- FORTRAN90 modularity and dynamic memory allocation (GWM);
- distributed memory multiprocessing for the entire energy range of all particles (GWM);
- repeated structures source-path improvement (LLC/JSH);
- default dose functions (LSW/JSH);
- light-ion recoil (JSH);
- enhanced color geometry plots (GWM/JSH);
- photonuclear cross-section plots (JSH);
- proton cross-section plots (JSH);
- proton reaction multipliers with FM cards (JSH);
- photonuclear reaction multipliers with FM cards (JSH/GWM);
- some speedups (GWM/JSH);
- logarithmic interpolation on input cards (JSH);
- cosine bins that may be specified in degrees (JSH);
- cosine bins that may be specified for F2 flux tallies (JSH);
- source particles that may be specified by descriptors (JSH);
- pause command for tally and cross-section plots (JSH); and
- correction of all known MCNPX and MCNP4C bugs/problems.

MCNPX 2.3.0 and previous MCNPX versions (1995–2001)

- physics for 34 particle types (HGH);
- high-energy physics above the tabular data range (REP);
- photonuclear physics (MCW);

- neutron, proton, and photonuclear 150-MeV libraries and utilization (RCL);
- mesh tallies (tallies in a superimposed mesh) (LSW/ECS);
- radiography tallies (JSH/ECS);
- secondary-particle production biasing (ECS); and
- autoconfiguration build system for compilation (TLR/HWE).

MCNP4C3, MCNP4C2, and MCNP4C features added after MCNP4B (1997–2001)

- PC enhancements: Linux and Windows capable (LLC/GWM);
- easier geometry specification with macrobodies (LLC);
- interactive geometry plotting (JSH);
- improved variance reduction with the superimposed mesh weight-window generator (TME/JAF/JSH);
- superimposed mesh plotting (JSH);
- delayed neutrons (CJW);
- unresolved resonance range probability tables (LLC/RCL);
- perturbations for material-dependent tallies (GWM/LLC/JSH);
- ENDF/B-VI extensions (MCW);
- electron physics enhancements (upgrade to ITS3.0)[2] (KJA/HGH);
- weight-window enhancements (JSH/JAF); and
- distributed memory multiprocessing (GWM).

1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay $20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new $2 bill for any error in MCNPX that has been inherited from its constituent codes.[3]

MCNPX is a better quality code than MCNP4C3. First, it corrects many MCNP4C3 problems. Second, cash awards have been earned less frequently with MCNPX than with MCNP4C3 and its predecessors. In the past 2 years, fewer than 20 MCNPX cash

---

[2] J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, M. J. Berger, "ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAND91-1634 (March 1992).

[3] Cash Award Fine Print: Offer subject to cancellation or modification without notice. A bug is defined as an error in the source code that we choose to correct. We make awards even for the most trivial or insignificant problems, but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We believe that MCNPX and its predecessor codes are the most error-free and robust Monte Carlo radiation transport capabilities, and we back them with a cash guarantee.

awards have been given. A listing of winners is available at http://mcnpx.lanl.gov. MCNPX bugs are described in the newsletter for each MCNPX version.

1.3. Availability

MCNPX 2.4.0 is available from the RSICC in Oak Ridge, Tennessee, USA, at http://www-rsicc.ornl.gov. MXNPX 2.4.0 is also available from the OECD NEA Data Bank in Paris, France, at http://www.nea.fr.

An essential part of the MCNPX software quality assurance plan is the beta test program. Before a code version goes to RSICC or OECD/NEA, it is made available to over 1000 MCNPX beta testers worldwide. MCNPX 2.5.c is available to beta testers on the MCNPX website at http://mcnpx.lanl.gov. To apply for a beta test password and to have access to the latest MCNPX versions, contact Laurie Waters at lsw@lanl.gov.

All beta test, RSICC, and OECD/NEA versions of MCNPX are guaranteed with cash awards.

2.0. USER INTERFACE FOR NEW MCNPX FEATURES

The new MCNPX capabilities involve numerous user interface changes from MCNP4C3 and older MCNPX (2.3.0 and earlier) versions. These changes mostly are extensions of existing input cards.

2.1. PHYS Changes

2.1.1. Neutrons

PHYS:N *EMAX EAN IUNR DNB TABL FISM RECL*

EMAX = upper energy limit (default = 100 MeV)
EAN = analog capture below *EAN;* implicit capture above EAN (default = 0 MeV)
IUNR = unresolved resonance range probability table treatment
    = 0/1 = on/off (default = 0) when unresolved data are available
DNB=delayed neutrons from fission.
    -1 = analog production of delayed neutrons from fission (default)
    0 = treat prompt and delayed neutrons as prompt
    n = biased production: produce up to n delayed neutrons per fission
        (n > 0 disallowed in KCODE)
TABL = use data tables below *TABL;* physics models above *TABL*
    = -1 (default) (Mix and Match) When tables are available, use them up to
        their upper limit and use physics models above.
FISM = fission multiplicity
    = 0 (default) MCNP treatment. The number of neutrons per fission is the
        integer above or below ν. If ν = 2.7, then the number of neutrons

will be two 30% of the time and three 70% of the time.
= FWHM : sample Gaussian with full-width half-maximum of FWHM about ν
= -1 : sample Gaussian with FWHM appropriate for fissioning nuclide (recommended)

RECL = light ion recoil. Produce 0 < *RECL* < 1 light ions (h, d, t, s, a) at each elastic scatter with light nuclei (H, D, T, ^{3}He, ^{4}He). The ionization potential is accounted for, and the proper two-body kinematics is used (with neutron free-gas thermal treatment if appropriate) to bank the created particles with the proper energy and angle. MODE n h d t s a … is required to produce 1 light ions (h, d, t, s, a). *CUT:x 2J 0* for x = h, d, t, s, a is recommended so that the low-energy recoil ions produced are not killed by energy cutoff.

2.1.2. Protons

PHYS:H *EMAX EAN TABL J ISTRG J RECL*

EMAX = upper energy limit (default = 100 MeV)
EAN = analog capture below *EAN;* implicit capture above EAN (default = 0 MeV)
TABL = use data tables below *TABL*; physics models above *TABL*
= -1 (default) (Mix and Match) When tables are available, use them up to their upper limit and use physics models above.
J = jump (unused)
ISTRG = charged particle straggling control
= 0 Vavilov (default, best)
= 1 Continuous slowing down approximation
= -1 old MCNPX 2.2.4 method
J = jump (unused)
RECL = light ion recoil. Produce 0 < *RECL* < 1 light ions (h, d, t, s, a) at each elastic scatter with light nuclei (H, D, T, ^{3}He, ^{4}He). The ionization potential is accounted for, and the proper two-body kinematics is used to bank the created particles with the proper energy and angle. MODE h d t s a … is required to produce light ions (h, d, t, s, a). *CUT:x 2J 0* for x = h, d, t, s, a is recommended so that the low-energy recoil ions produced are not killed by energy cutoff. Note that protons colliding with hydrogen to produce more protons can produce an overwhelming number of protons; caution is required and *RECL < 1* may be needed.

2.1.3. Charged Particles

PHYS:x *EMAX 3J ISTRG*

EMAX = upper energy limit (default = 100 MeV)
J = jump (unused)
ISTRG = charged particle straggling control
= 0 Vavilov or Prael's new straggling model, which is an energy correction addressing stopping powers. (default, best)

= 1 Continuous slowing down ionization model
= -1 old MCNPX 2.2.4 method

2.2. MX Card: Mix-and-Match Nuclide Replacement

The new MCNPX MX card enables materials substitution for different particle types. It is an extension of, and replacement for, the MPN card for photonuclear data:

MXn:p zaid1 zaid2 ...

where n = material number of an Mn card that MUST precede the MXn card;
p = particle type (n, p, h)

zaidn = replacement nuclide for the nth nuclide on the Mn card.

Only particle types n (neutron), p (photonuclear), and h (proton) are allowed on the MX card. No substitutions are allowed for photoatomic (p) and electron (e) data because those data sets are complete. The MXn:P card is an exact replacement of the MPNn card and specified photonuclear nuclide substitutions (library type u). zaidn = 0 is allowed on MXn:P (photonuclear substitution) to specify no photonuclear data for a specific photoatomic reaction. zaidn = model is allowed on the MXn:N and MXn:H (neutron and proton substitution) to allow models to be mixed with tabular data. As an example, consider the following input file:

```
mode n h p
phys:p 3j 1
m1        1002 1    1003.6 1   6012 1   20040  1    nlib .24c
mx1:n j   model     6000       20000
mx1:h     model     1001       j        j
mpn1      6012      0          j        j
```

MCNPX will issue the following warnings:

```
warning. MPNn will soon be obsolete. use MXn:p instead.
warning. photonuclear za = 6012 different from nuclear za = 1002
warning. photonuclear za =   0 different from nuclear za = 1003
```

Note that models will be used for neutron tritium and proton deuterium. The MPN card still works but has a warning. The mixing and matching is summarized in Print Table 101:

```
1particles and energy limits                                                    print table 101

                    particle    maximum     smallest    largest     always use   always use
                    cutoff      particle    table       table       table        model
particle type       energy      energy      maximum     maximum     below        above
```

1	n	neutron	0.0000E+00	1.0000E+37	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02
2	p	photon	1.0000E-03	1.0000E+02	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05
9	h	proton	1.0000E+00	1.0000E+02	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02

2.3. COINC Card: ^{3}He Coincidence Modeling

Helium-3 coincidence detectors now may be modeled using the new COINC card and fission multiplicity (PHYS:N card, sixth entry). The COINC card is

COINC i1 i2 … ,

where i1, i2, … are cell numbers of ^{3}He coincidence counting cells. For each cell listed, the captures and moments will be output in Print Table 118:

```
1neutron captures on helium-3, moments and multiplicity distributions by cell.  print table 118

 cell  23:

 neutron captures on 3he
                         captures      captures            multiplicity fractions
            histories   by number     by weight      by number        by weight      error

 captures = 0     7784         0      0.00000E+00     7.78400E-01     7.78400E-01    0.0053
 captures = 1     1586      1586      1.58600E-01     1.58600E-01     1.58600E-01    0.0230
 captures = 2      370       740      7.40000E-02     3.70000E-02     3.70000E-02    0.0510
 captures = 3      167       501      5.01000E-02     1.67000E-02     1.67000E-02    0.0767
 captures = 4       51       204      2.04000E-02     5.10000E-03     5.10000E-03    0.1397
 captures = 5       20       100      1.00000E-02     2.00000E-03     2.00000E-03    0.2234
 captures = 6       10        60      6.00000E-03     1.00000E-03     1.00000E-03    0.3161
 captures = 7        4        28      2.80000E-03     4.00000E-04     4.00000E-04    0.4999
 captures = 8        5        40      4.00000E-03     5.00000E-04     5.00000E-04    0.4471
 captures = 9        2        18      1.80000E-03     2.00000E-04     2.00000E-04    0.7070
 captures = 11       1        11      1.10000E-03     1.00000E-04     1.00000E-04    0.9999

total            10000      3288      3.28800E-01     1.00000E+00     1.00000E+00    0.0235

     factorial moments              by number                 by weight

           3he                  3.28800E-01  0.0235      3.28800E-01  0.0235
       3he(3he-1)/2!            1.87800E-01  0.0732      1.87800E-01  0.0732
   3he(3he-1)(3he-2)/3!         1.52400E-01  0.1719      1.52400E-01  0.1719
 3he(3he-1) .... (3he-3)/4!     1.37300E-01  0.3026      1.37300E-01  0.3026
 3he(3he-1) .... (3he-4)/5!     1.15800E-01  0.4428      1.15800E-01  0.4428
 3he(3he-1) .... (3he-5)/6!     8.08000E-02  0.5956      8.08000E-02  0.5956
 3he(3he-1) .... (3he-6)/7!     4.46000E-02  0.7497      4.46000E-02  0.7497
 3he(3he-1) .... (3he-7)/8!     1.88000E-02  0.8803      1.88000E-02  0.8803
 3he(3he-1) .... (3he-8)/9!     5.70000E-03  0.9652      5.70000E-03  0.9652
 3he(3he-1) .... (3he-9)/10!    1.10000E-03  0.9999      1.10000E-03  0.9999
 3he(3he-1) .... (3he-10)/11!   1.00000E-04  0.9999      1.00000E-04  0.9999
```

Coincidence counting works only for neutron problems run in a completely analog mode with fission multiplicity and analog capture (PHYS:N J 100 3J –1) or CUT:N 2J 0 0) and NO variance reduction. The ^{3}He captures and moments can be compared to Print Table 117, which has the spontaneous fission source and induced fission summaries of fission neutrons and moments.

2.4. SDEF Source Specifications

2.4.1. Particle-Type Specification
The source particle type now may be specified on the SDEF card by its symbol

```
SDEF PAR = h    .
```

2.4.2. Positron Sources
Positron sources may now be specified as

```
SDEF PAR = -e  or SDEF PAR = -3   .
```

Note that positron physics in MCNPX, just as with MCNP and the Integrated Tiger Series (ITS), is identical to electron physics except for positron annihilation. Electrons below the energy cutoff are terminated, whereas positrons below the energy cutoff produce annihilation photons. Also, the positrons have a positive charge and may be tallied using the FT card ELC option.

2.4.3. Repeated Structures Source Specifications
The CEL source specification for repeated structures geometries is now consistent with the tally specification. The old MCNP4C specification still works, but the new one is

```
SDEF CEL=d3 POS=0 6 0 EXT=d1 RAD=d2 AXS= 0 1 0
SI3 L (1<10[0 0 0]<11) (1<10[1 0 0]<11) (1<10[2 0 0]<11)
        (1<10[0 1 0]<11) (1<10[1 1 0]<11) (1<10[2 1 0]<11)   .
```

2.4.4. Spontaneous Fission Sources
Spontaneous fission may be specified as a source:

```
SDEF PAR = sf CEL = …   .
```

Eighteen nuclides are available: ^{232}Th, ^{232}U, ^{233}U, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242}Cm, ^{244}Cm, ^{249}Bk, and ^{252}Cf.

Cells are sampled according to the usual SI and SP distributions. If more than one spontaneous fission nuclide is in a source cell, the fissioning nuclide will be chosen proportionately to the product of its atom fraction and the spontaneous fission yield for each nuclide. If no spontaneous fission nuclide is found in a specified source cell, the code exits with a bad trouble error, "spontaneous fission impossible.”

The number of spontaneous fission neutrons then is sampled. The spontaneous fission multiplicity data of Ensslin is used. The energies are sampled from a Watt spectrum with appropriate spontaneous fission parameters for the selected nuclide. Currently, only the first spontaneous fission neutron from each history is printed. If the spontaneous fission samples a multiplicity of zero—that is, no neutrons for a given spontaneous fission—then the history is omitted from the first 10 history lists of Print Table 110. The number of source particles is the number of spontaneous fission neutrons, which will be ν times the requested number of source histories on the NPS card. Currently, all summary and tally normalization is done by source histories, which is the number of spontaneous fissions, not the number of spontaneous fission neutrons.

Fission multiplicity for induced fissions (6h entry, PHYS:N card) automatically is turned on with the default width (FISM = -1 = nuclide dependent). If FISM > 0 on the PHYS:N card, then that value will be used. Multiplicity and moments are printed in Print Table 117 for both spontaneous and spontaneous plus induced fissions.

2.5. Tallies

2.5.1. Expanded Cosine Specification

Cosines now may be specified in degrees. They now also may be specified with flux tallies as

    *C2 150 120 90 60 30 0   .

The * on the C2 card interprets cosines as in degrees. Entries must be such that the cosine is monotonically increasing.

2.5.2. DF Card: Default Dose Functions

The DE/DF dose function cards are unchanged but now have extensions. As before, dose conversions may be input as a table. Note that the interpolation int = log or int = lin now may be placed anywhere, and n = tally number, which implies particle type.

    DEn E1 E2 int E3 ...
    DFn F1 int F2 F3 ...

The dose conversion capability is extended to provide standard default dose functions. These are invoked by omitting the DE card and using keywords on the DF card:

    DFn iu=j fac=F int ic=I   ,

where the following entries are all optional:

iu = 1 = US units (rem/h)
iu = 2 = international units (sieverts/h)
Default: iu = 2 international units (sieverts/h)

fac = normalization factor for dose (acr is also accepted instead of fac).

fac = -1 = normalize results to Q = 20 by dividing the parametric form of Q [5.0+17.0*exp(-(ln(2E))*2/6)] from ICRP60 (1990), paragraph A12.
fac = -2 = apply LANSCE albatross response function.
Default: fac = 1.0.

int = "log" or "lin" results in "log" or "lin" interpolation of energy; the dose function is always linear. That is, "lin" results in "linlin" interpolation, and "log" results in "loglin" interpolation.

Default: for ic = 10, 40: log
for ic = 20,31-39: recommended analytic parameterization.

ic = i = standard dose function.

<u>i neutron dose function</u>
10 = ICRP-21 1971
20 = NCRP-38 1971, ANSI/ANS-6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 (AP anterior-posterior)
32 = (PA posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
40 = ICRP-74 1996 ambient dose equivalent

<u>i photon dose function</u>
10 = ICRP-21 1971
20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1977
31 = ANSI/ANS-6.1.1-1991 [AP (anterior-posterior)]
32 = PA (posterior-anterior)
33 = (LAT side exposure)
34 = (ROT normal to length and rotationally symmetric)
35 = (ISO isotropic)

Default: ic = 10

Examples:

DF4

DF0 ic 40 iu 1 lin fac 123.4

DF1 iu=2 acr=-2 log ic=34

2.5.3. Photonuclear and Proton Reaction Multipliers

Photonuclear and proton cross sections may be used in tally multipliers on the FM card. For example,

```
M102 92235 1 pnlib=27u
F2:P 1
FM2    (-1 102 18 1018)
```

Photonuclear cross-section reaction numbers are all positive, unlike the photoatomic reaction numbers, which are negative. The principal photonuclear cross sections are the following: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, and >4 = various reactions such as 18 = (γ,f). The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 times the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); and 1018 is the total number of neutrons (particle type n = 1) from fission.

Proton reaction numbers are similar to the neutron reaction numbers: all positive. The principal proton cross sections are the following: ±1 = total, ±2 = nonelastic, ±3 = elastic, ±4 = heating, >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers are specified by adding 1000 times the secondary particle number to the reaction number. For interaction reaction mt = 5, the multiplicities are 1005 for neutrons, 9005 for protons, 31005 for deuterons, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available, along with the total cross-section and heating number, mt = 1, mt = 4.

It is always wise to plot the desired cross sections first to see if they are available with the expected reaction numbers in the data library. The tally multipliers treat the data the same as the data are treated in transport: the cross section at the lowest energy is extended down to E = 0 for protons with mt < 0; the cross section at the highest energy of the table is extended to E = ∞ for proton interaction cross sections with mt < 0, and for photonuclear interaction cross sections, mt < 1000. These extrapolations can be seen in the cross-section plots.

2.6. Geometry Plots

The new plotting capabilities are accessible via either the interactive geometry plot capability or the command/prompt interface.

2.6.1. I,J,K Lattice Index Labeling

The i,j,k lattice indices of repeated structures/lattice geometries now may be used as plot labels in geometry plots, as illustrated in Fig. 1.

If the level (LEVEL command or button) is not a lattice cell level, then the indices will be for the next lattice in a higher level. To get the lattice index labels, choose ijk as the edit quantity by clicking ijk in the right margin. Then click the send entry after LABEL so that it reads “LABEL off ijk”. For command/prompt plotting, enter “Label 0 1 ijk”.

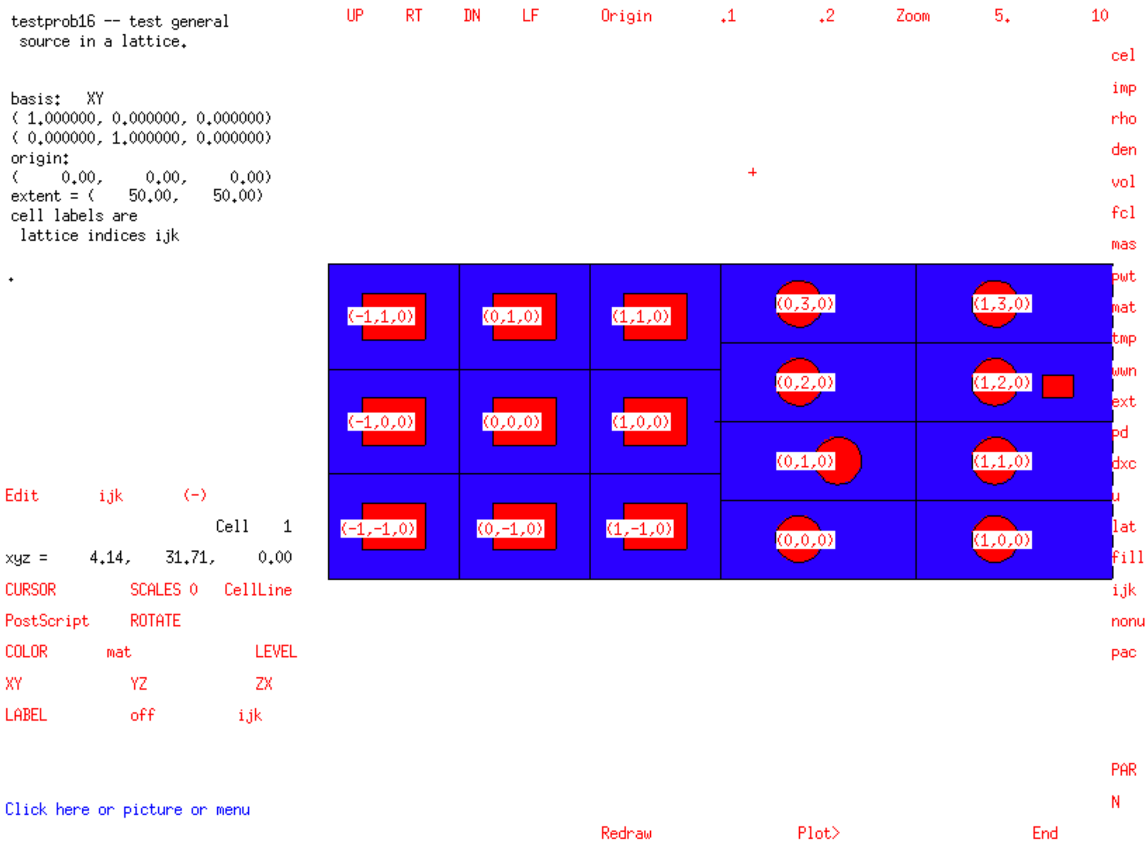

Fig. 1. Lattice indexing in geometry plot.

2.6.2. Sixty-Four-Color Plotting and Coloring by Cell Parameters

MCNP4C3 has 7 plotting colors; MCNPX now has 64-color plotting. Coloring of geometry plots may be used for any cell parameter. MCNP4C colored its geometry plots by material only, giving a different color to each material number. MCNPX now can color geometry plots by any cell quantity. Each cell can have a different color, or each repeated structure level or universe can have a different color. Logarithmic shading of importances, weight windows, and summary information is automatic. If a superimposed weight-window mesh is used, coloring also may be done by the value of the mesh weight windows.

In the interactive capability, the “SCALES n” button has been moved up two lines (after the cursor) to make room for a larger “COLOR name” button. The default is “COLOR mat”, which colors problem cells by the program material number. This button must be clicked to get “COLOR off” (black and white) and then clicked again to color by whatever parameter is listed after the “Edit” button. For example, in the right margin, click “cel”, which will make the “Edit” quantity “cel”. Next, click “COLOR” so that it says "COLOR cel"; on the next plot, the color shades will be determined by program cell number.

For command/prompt plotting, enter

PLOT> label 0 1 rho ;

the color command then must be set such as

PLOT> color on ,

and the coloring will now be by rho, the atom density.

2.7. Tally and Cross-Section Plots

2.7.1. Pause Command

The MCNPX geometry plot *PAUSE* command now is extended to tally and cross-section plots. When the word *PAUSE N* is put in a tally plotting the COM input file, the picture will display for *N* seconds. If the command *PAUSE* (without the *N*) is in the COM file, the display will hold until a key is struck.

2.7.2. Photonuclear Cross-Section Plots

MCNPX can plot photonuclear data in addition to the photoatomic data of MCNP.

Photoatomic reaction numbers are all negative: -1 = incoherent, -2 = coherent, -3 = photoelectric, -4 = pair production, -5 = total, and -6 = heating. For the MCNPX photonuclear cross-section plotting, the reaction numbers are all positive. The principal photonuclear cross sections are as follows: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, and >4 = various reactions such as 18 = (γ,f). The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 times the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); and 1018 is the total number of neutrons (particle type n = 1) from fission. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available photonuclear reactions and the available yields such as 1018, 31018, 34018. Entering a bad nuclide, xs = 12345.67u, will cause MCNPX to list the available nuclides.

Figure 2 illustrates a photonuclear cross-section plot of the total photonuclear cross section, mt = 1, for material 11 and its constituents, carbon and lead.

2.7.3. Proton Cross-Section Plots

MCNPX now can plot proton cross sections. The reaction numbers are similar to the neutron reaction numbers: all positive. The principal proton cross sections are the following: ±1 = total, ±2 = nonelastic, ±3 = elastic, ±4 = heating, and >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 with its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers for interaction reaction mt = 5 are 1005 for neutrons, 9005 for protons, 31005 for deuterons, etc. To

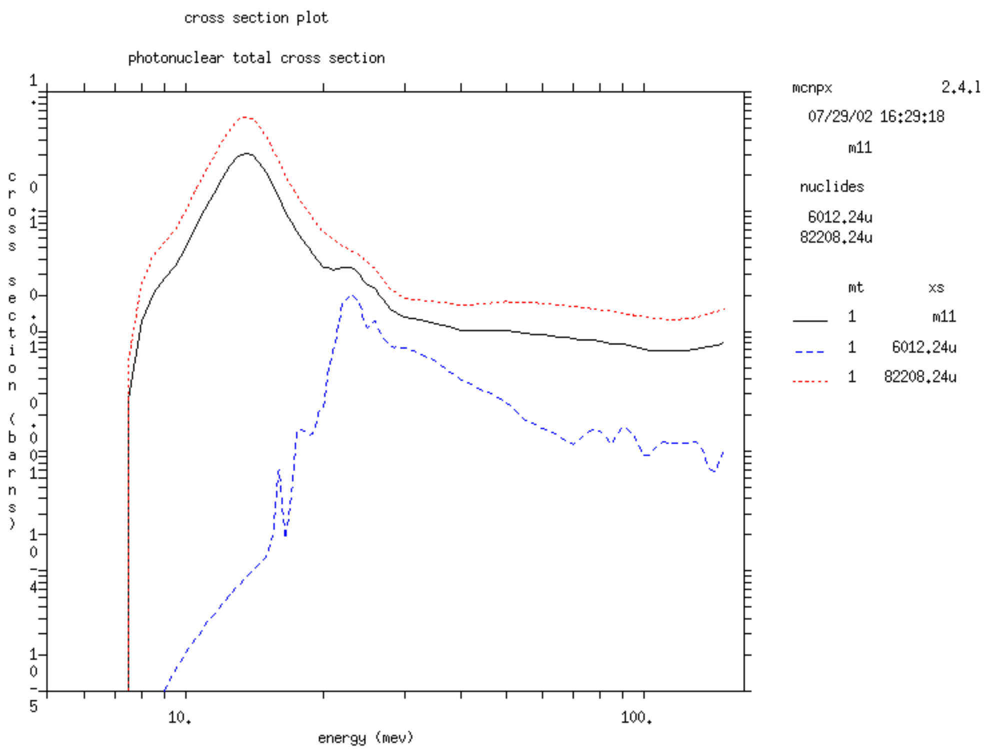

Fig. 2. Photonuclear cross-section plot.

find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available proton reactions and the available yields such as 1005, 32001, and 34002. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available, along with the total cross-section and heating number, mt = 1, mt = 4. Entering a bad nuclide, xs = 12345.67h, will cause MCNPX to list the available proton nuclides.

2.7.4. Annoying Bell

The bell that "beeped" when plots were finished has been disabled. In ancient times, getting plots up on the screen took forever, and so the bell announced that the plot was ready. Now plotting is so fast that the bell is annoying and unneeded.

2.8. Other Capabilities

2.8.1. Logarithmic Interpolation

Logarithmic interpolation is now allowed on all input cards where lists of numbers are given. It is similar to the IJMR interpolation. For example,

E0 1.e-3 6log 1.e4

is interpreted as

E0 .001 .01 .1 1 10 100 1000 10000 .

2.8.2. Changes in Installation/Compilation

The autoconfiguration has been upgraded significantly for MCNPX installation and compilation. F90 is now the default, so on Unix systems it is no longer necessary to configure with

configure –with-FC=f90 –with-CC=cc .

Instead, simply enter

configure .

2.8.3. MPI Multiprocessing

To compile MCNPX with MPI, it is necessary to use the new "MPI" compilation/ configuration directive:

Configure –with-MPILIB[="/path/to/MPI/libraries -lmpich"] .

To run an MCNPX problem with MPI, simply start the MPI daemon (which typically is running already on most systems) and then start MCNPX using "MPIRUN". An example is

mpirun -np 4 mcnpx inp=gwm na=gwm1. ... .

This is quite different from the parallel virtual machine (PVM), which required knowledge about setting certain links, environment variables, and the PVM console commands. An example of the PVM execution command is

mcnpx inp=gwm n=gwm1. tasks=-12 .

3.0. DESCRIPTION OF NEW MCNPX 2.5.C FEATURES

The principal MCNPX 2.5.c new features are

- MPI multiprocessing (JL/GWM);
- i,j,k lattice indexing in geometry plots (JSH),
- enablement of the weight-window generator in the physics model region (FXG/JSH);
- enablement of the exponential transform in the physics model region (FXG/ JSH);
- extension of the neutron model physics below 20 MeV (JSH);
- ^{3}He coincidence detector modeling (HGH/JSH);
- F90 autoconfiguration (TLR); and

- corrections/enhancements/extensions.

3.1. MPI Multiprocessing

MCNPX now supports distributed memory multiprocessing for the entire energy range of all particles with both PVM and MPI. MPI is the standard from Argonne National Laboratory (ANL). A portable version called MPICH is available at http://www-unix.mcs.anl.gov/mpi/. PVM is the standard from Oak Ridge National Laboratory, available at http://www.csm.ornl.gov/pvm/pvm_home.html/.

Testing to date on a Linux cluster shows that the MPI version of MCNPX is slightly slower than that of the PVM; however, MPI can make use of the native high-speed interconnects (e.g., Myrinet) rather than just Ethernet. PVM cannot make use of these speedy interconnects because it is forced to use TCP/IP.

The MCNPX 2.5.c MPI implementation includes dynamic buffering. This is a significant advantage over PVM, which uses a fixed buffer size (the PVM buffer size is controlled with an environment variable—which most people know nothing about). The initial buffer size is set to 10 Mb and the maximum number of increases is 10, resulting in an upper limit of 100 Mb. These values are set via parameters that are modified easily in module MESSAGE_PASSING. MPI enables parallel computations on PC Windows. PVM does not yet support Windows 2K.

The MPI version of MCNPX requires only “freeware” software, as did PVM. The MPICH product can be downloaded from ANL and installed on either Windows or Unix platforms. On Unix platforms, care must be taken to produce F90 versions of the libraries and not the default Fortran 77 ones. On Windows, users do not even need to build the MPI libraries because they can simply download and install the prebuilt ones. So far, the MPI version of MCNPX has been tested on Linux, SGI, DEC, and Windows PC.

3.2. I,J,K Lattice Indexing in Geometry Plots

It is now possible to label repeated structures/lattices with their i,j,k indices in geometry plots (see Section 2.6.1).

3.3. Weight-Window Generator Improvements

The weight-window generator variance-reduction capability has been extended to the MCNPX physics model region for both neutral and charged particles. Both cell-based and mesh-based weight windows now can be generated for high-energy problems.

MCNPX now allows cell-based weight windows and importances to be used in conjunction with mesh-based weight windows. Previously, all WWINP file weight windows had to be used if available; otherwise, importances were used. Now WWINP weight windows are used only if the fifth WWP entry is negative; otherwise, cell-based windows or importances from the input file are used. In particular, if a mesh-based window is bad in the WWINP file, it may now be ignored and importances or cell-based windows from the input file may be used instead.

Whenever multigroup weight windows are generated, MCNP and MCNPX generate a one-group weight-window file as well, WWONE. Now the WWONE file includes one-group windows for all particles regardless of how many weight-window generator groups, if any, those particles had. Previously, the WWONE file was worthless if some particles generated one-group windows and other particles generated multigroup windows.

3.4. Exponential Transform in Physics Model Region

The exponential transformation variance reduction technique is now available for neutral particles in the physics model region of MCNPX. Note that the exponential transform should not be used without weight windows.

3.5. Extend Neutron Model Physics below 20 MeV

MCNPX now may use neutron models below 20 MeV. This is useful for nuclides where there is no table data, such as germanium in a bismuth germinate (BGO) particle detector. It is also useful for running pulse height tallies and other analog problems where data table (n,2n) reactions are not correlated, whereas the model physics reactions are all correlated. Finally, it is useful for comparing the models to the data tables. A major report is now available comparing physics model and data table results as part of the mix-and-match documentation.[4]

3.6. ^{3}He Coincidence Detector Modeling

MCNPX now has a ^{3}He neutron coincidence detector model (see Section 2.3). It works in conjunction with fission multiplicity and analog capture (see Section 2.2.1) and optionally with spontaneous fission sources (see Section 2.4.4).

Multiplicity counting[5] is a nondestructive assay technique for fissionable materials. Neutron coincidence counting looks for groups of neutrons that are close together in time, within the coincidence resolving time or "gate width" of the electronics package. In practice, multiplicity data analysis is not based directly on the observed multiplicity

[4] John S. Hendricks, "MCNPX Model/Table Comparison," Los Alamos National Laboratory report LA-14030 (March 2003).

[5] N. Ensslin, W. C. Harker, M. S. Krick, D. G. Langner, M. M. Pickrell, and J. E. Stewart, "Application Guide to Neutron Multiplicity Counting," Los Alamos National Laboratory report LA-13422-M (November 1998).

distribution but on the moments of the distribution. The factorial moments, ν_k, of a neutron multiplicity distribution emitted by a multiplying sample are [6,7]

$$\nu_1 = \sum \nu \, P(\nu) \; , \; \nu = 1 \, , \, \max$$

$$\nu_2 = \sum \nu \, (\nu - 1) \, P(\nu) \; , \; \nu = 2 \, , \, \max$$

$$\nu_3 = \sum \nu \, (\nu - 1) \, (\nu - 2) \, P(\nu) \; , \; \nu = 3 \, , \, \max$$

$$\nu_k = \sum \nu! \, P(\nu) \; / \; (\nu - k)! \; , \; \nu = k \, , \, \max \; .$$

The MCNPX fission multiplicity and ^3He coincidence counting capabilities of MCNPX enable direct comparisons with measurements.

Fission multiplicity in MCNPX samples the correct number of fission neutrons to emerge from a fission event. Previous MCNPX/MCNP versions simply emitted the nearest number of fission neutrons to ν_{avg} . Thus, for ν_{avg} = 2.7, two neutrons would be emitted 30% of the time and three neutrons would be emitted 70% of the time. Now the correct number, from 0 to 11, of fission neutrons is emitted at each fission and both the multiplicity distribution and moments are tabulated for all fissions. The number of fission neutrons from each fission event is sampled from the appropriate Gaussian distribution about ν_{avg} .

The coincidence counting model simply counts the analog capture of neutrons by ^3He in geometric cells specified on the COINC card. These captures then are tabulated along with the capture moments. Comparison of the capture moments and fission multiplicity moments enables comparison with measurements.

The following table compares MCNPX calculations to measurements for Californium sources in an Epithermal Neutron Multiplicity Counter (ENMC). The table shows a straight comparison between counting rates for singles, doubles, and triples (moments). The experimental values have been corrected for dead time and gate width.

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[6] K. Boehnel, "The Effect of Multiplication on the Quantitative Determination of Spontaneously Fissioning Isotopes by Neutron Correlation Analysis," *Nuclear Science and Engineering,* **91,** 114 (1985).

[7] W. Hage and D. M. Cifarreli, "Correlation Analysis with Neutron Count Distributions in Randomly or Signal Triggered Time Intervals for Assay of Special Nuclear Materials," *Nuclear Instruments and Methods,* **A236,** 165 (1985).

3.7. Fortran90 Autoconfiguration

The MCNPX autoconfiguration code installation and compiling capability has been significantly revised. The F90 compiler is now the default on all platforms and it is no longer necessary to declare F90 at the configure step (see Sections 2.8.2 and 2.8.3). The directories and compile directives have been revised to prepare for the imminent

Comparison of Measurement/MCNPX MCNPX-Calculated Count Rates						
	S		D		T	
Cf-10	159835		99959		37075	
Cf-11	296568		185470		68792	
Cf-12	567456		354881		131627	
ENMC Measured Rates						
Cf-10	160788		100573		36426	
Cf-11	297647		186006		68173	
Cf-12	569117		355386		130467	
Measurement/Calculation						
Cf-10	1.0060		1.0061		0.9825	
Cf-11	1.0036		1.0029		0.9910	
Cf-12	1.0029		1.0014		0.9912	
Average	1.004		1.003		0.988	
St. Dev.	0.002		0.002		0.005	

integration of the Intra Nuclear Cascade Liege (INCL) (Cugnon/Schmidt) physics model.

F90 provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. F90 will run more slowly on some systems. Specifically, we have eliminated equivalences as a means of dynamic storage allocation by using F90 pointers and allocable arrays. We have replaced most common calls with F90 modules. The code will compile in both free and fixed F90 formats.

MCNPX can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX .

Continuing improvements in the F90 structure are ongoing, especially where they concern physics modules that have been brought into the code.

3.8. Corrections/Enhancements/Extensions

3.8.1. Some Significant Problems

The following problems could cause wrong answers.

3.8.1.1. Dynamic Memory Allocation Error

The following problems have occurred with some compilers on some systems, notably the Sun Solaris Forte 6.2 compiler:

- compilation errors preventing compilation;
- inability to continue runs; and
- overwriting of memory.

Consequently, we have reallocated dynamic memory to prevent arrays from ever having zero length. Evidently, zero-length arrays have always been possible on older compilers and systems.

3.8.1.2. Physics Model Heating Wrong

In all previous versions of MCNPX (and probably LAHET as well), the heating in the physics model energy range only is multiplied by the particle weight squared. Thus, if the weight is not exactly one, then the heating is wrong. Fortunately, most problems use a source weight of one, and there is seldom variance reduction in the physics model region. To see if your problems were affected, try a source weight of SDEF WGT = 1000. If your heating tallies increase by a factor of 1000, then the code is functioning correctly. If they increase by a factor of 1,000,000, then this bug affected you.

3.8.1.3. Light-Ion Recoil Errors

In previous versions, light-ion recoil was off by a factor of the atomic weight ratio. Thus recoil of protons was correct, but recoil of other light ions was wrong. Twenty dollars was awarded to Martyn Swinhoe (LANL, NIS-5) (D-10:JSH-2003-034). Also, light-ion recoil bias, when RECL on the PHYS:N card seventh entry was not 0 or 1, resulted in wrong particle weights. Twenty dollars was awarded to Martyn Swinhoe (NIS-5) (D-10:JSH-2003-030).

3.8.1.4. Mesh Tally Options

Mesh tally options were ignored on mesh tally cards with particle-type designators, i.e., cmesh1=n flux trans 1 (FXG).

3.8.1.5. MDATA Binary Files for Mesh Tallies

The binary format MDATA file used to make mesh-tally plots was improperly normalized in KCODE and SSR problems. Twenty dollars was awarded to Bernard Verboomen (SCI-CEN, Belgium) (D-10:JSH-2003-036).

3.8.2. Irritating Problems

The following problems do not cause wrong answers. In some cases MCNPX will crash, and in others the desired functionality simply is absent.

3.8.2.1. SPABI Failure

The secondary particle production biasing (SPABI) capability simply did not work for some compilers because an integer function had a floating point name. Answers were correct, just not biased as desired. Also, all previous MCNPX versions put SPABI roulette in the "photon production from neutrons" summary table bin, which usually caused unbalanced summary tables. Now the roulette shows up in "energy importance" for all particles.

3.8.2.2. 32-Bit SGI Compiler Error

An error in some compilers for 32-bit SGI machines caused an out-of-range error. We have built in a workaround in MCNPX, even though this is an SGI error that causes a crash, not an MCNPX error.

3.8.2.3. Occasional Crashes for Some Data Libraries

MCNPX sometimes crashed if angular distributions from the nuclear data tables were in tabular format. The crash occurred for only certain data libraries in certain energy regimes.

3.8.2.4. Cascade Exciton Model (CEM) Fails for Light Nuclei

CEM goes into an infinite loop for light nuclides, $A < 5$. MCNPX25c is changed to use Bertini for $A < 5$ and CEM for $5 < A < 10$ (though Stepan Mashnik says CEM should not be used for $A < 10$). Photonuclear production is now turned off for $A < 5$.

3.8.2.5. Gridconv Typo

When running the auxiliary program GRIDCONV to generate mesh tallies, the incorrect question "Do you what" was changed to "Do you want" in the user interface.

3.8.3. Enhancements

The following enhancements were made to MCNPX 2.5.c in addition to the major new capabilities listed above.

3.8.3.1. Spontaneous Fission, Fission Multiplicity, and ^{3}He Coincidence

- The source weight in the summary table and first 50 histories printed in Print Table 110 are fission neutrons, not fissions.

- The summary of spontaneous fission and induced fission multiplicity, Print Table 117, computes and lists the estimated error.

- The summary of ^{3}He capture, Print Table 118, computes and lists the estimated error.

- Spontaneous fission has been extended from 6 to 18 fission nuclei.

3.8.3.2. Enabling More Histories

An integer overflow has been fixed so that more histories can be run. With the new MPI and PVM parallel capabilities, more and more particles are being run.

3.8.3.3. CEM and LEB

The LEB input card parameters could not be increased when running with CEM. Two dollars was awarded to Paul Goldhagen, USDOE (New York) (D-10:JSH-03-015).

4.0. FUTURE WORK

- INCL (Cugnon/Schmidt) physics model.
- Plotting of physics model total and absorption cross sections.
- Special features for space applications.
- Forced collisions for neutral particles extended to physics models.
- Secondary particle angle biasing for isotropic distributions.
- Improved high-energy physics with the LAQGSM model.
- Multiple-source particle types.
- Pulse height tallies with variance reduction.
- Neutral particle perturbation techniques extended to physics model region.
- Interactive tally and cross-section plotting.
- Detectors and DXTRAN for all neutral particles at all energy ranges.
- A capability to continue runs that write HTAPE files.
- Integration of HTAPE tallies directly into MCNPX.
- Heavy-ion tracking and interactions.

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